Benzenamine, 2,4-dimethyl-

Other names:	1-AMINO-2,4-DIMETHYLBENZENE
	2,4-DIMETHYLANILINE
	2,4-Dimethylbenzenamine
	2,4-Dimethylbenzeneamine
	2,4-Dimethylphenylamine
	2,4-XYLIDINE
	2,4-Xylylamine
	2-Methyl-p-toluidine
	4-Amino-1,3-dimethylbenzene
	4-Amino-1,3-xylene
	4-Amino-3-methyltoluene
	4-Methyl-o-toluidine
	Aniline, 2,4-dimethyl-
	M-XYLIDINE
	NSC 7640
	m-4-Xylidine
Inchi:	InChI=1S/C8H11N/c1-6-3-4-8(9)7(2)5-6/h3-5H,9H2,1-2H3
InchiKey:	CZZZABOKJQXEBO-UHFFFAOYSA-N
Formula:	C8H11N
SMILES:	Cc1ccc(N)c(C)c1
Mol. weight [g/mol]:	121.18
CAS:	95-68-1

Physical Properties

Property code	Value	Unit	Source
af	0.4970		KDB
chl	-4655.50	kJ/mol	NIST Webbook
gf	176.08	kJ/mol	Joback Method
hf	38.93	kJ/mol	Joback Method
hfl	-88.70	kJ/mol	NIST Webbook
hfus	14.94	kJ/mol	Joback Method
hvap	47.64	kJ/mol	Joback Method
ie	7.65 ± 0.05	eV	NIST Webbook
ie	7.40 ± 0.10	eV	NIST Webbook
log10ws	-2.06		Crippen Method
logp	1.886		Crippen Method
mcvol	109.800	ml/mol	McGowan Method

pc	4000.00	kPa	KDB
rinpol	1131.00		NIST Webbook
rinpol	1123.10		NIST Webbook
rinpol	196.10		NIST Webbook
rinpol	196.10		NIST Webbook
rinpol	1167.01		NIST Webbook
rinpol	1145.70		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1123.10		NIST Webbook
rinpol	1137.70		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1160.70		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1976.00		NIST Webbook
tb	491.20	K	NIST Webbook
tb	487.45 ± 0.50	K	NIST Webbook
tb	490.27	K	KDB
tc	714.00	K	KDB
tf	258.90 ± 1.00	K	NIST Webbook
tf	261.05 ± 0.30	K	NIST Webbook
tf	259.32 ± 0.80	K	NIST Webbook
tf	259.35 ± 0.35	K	NIST Webbook
tf	257.25 ± 1.00	K	NIST Webbook
tf	289.00	K	KDB
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.15	J/mol×K	679.65	Joback Method
cpg	228.80	J/mol×K	491.61	Joback Method
cpg	240.98	J/mol×K	529.22	Joback Method
cpg	252.48	J/mol×K	566.83	Joback Method
cpg	263.33	J/mol×K	604.43	Joback Method
cpg	273.54	J/mol×K	642.04	Joback Method
cpg	292.16	J/mol×K	717.26	Joback Method
hvapt	61.30 ± 0.60	kJ/mol	317.00	NIST Webbook
hvapt	55.50	kJ/mol	434.00	NIST Webbook
hvapt	56.90	kJ/mol	405.50	NIST Webbook
rhol	969.46	kg/m3	293.10	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44845e+01
Coeff. B	-4.09072e+03
Coeff. C	-7.65780e+01
Temperature range (K), min.	364.72
Temperature range (K), max.	522.53

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.53270e+02
Coeff. B	-1.27469e+04
Coeff. C	-2.03281e+01
Coeff. D	1.36820e-05
Temperature range (K), min.	294.15
Temperature range (K), max.	473.15

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C95681&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1306

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/files/research/kdb/mol/mol1306.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume